LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081821\
Data File : BP006745.D
Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.858	297	301	306	rVB	76333	110654	1.27%	0.192%
2	5.305	371	377	388	rVB	3248878	4602848	52.79%	7.985%
3	6.887	639	646	659	rVB	3090116	4774402	54.76%	8.282%
4	7.699	778	784	792	rVB	742434	1128179	12.94%	1.957%
5	8.858	974	981	991	rBV	1927216	3154809	36.18%	5.473%
6	10.281	1217	1223	1239	rBV	650631	1165801	13.37%	2.022%
7	10.481	1250	1257	1265	rBV	939779	1550263	17.78%	2.689%
8	12.963	1672	1679	1692	rBV	4374318	6198788	71.10%	10.753%
9	13.251	1721	1728	1736	rBV	212552	333058	3.82%	0.578%
10	14.063	1861	1866	1874	rVB	70900	114003	1.31%	0.198%
11	14.340	1904	1913	1920	rBV	1305143	1927378	22.11%	3.344%
12	15.316	2073	2079	2088	rBV5	47301	89905	1.03%	0.156%
13	15.840	2162	2168	2179	rVB	3572444	4888108	56.06%	8.480%
14	17.098	2376	2382	2386	rBV	1591636	2251833	25.83%	3.906%
15	17.140	2386	2389	2397	rVV	347927	506423	5.81%	0.879%
16	17.234	2397	2405	2411	rVB	117771	194840	2.23%	0.338%
17	17.516	2443	2453	2462	rBV	46034	120609	1.38%	0.209%
18	17.792	2496	2500	2513	rVB	151240	214340	2.46%	0.372%
19	17.975	2525	2531	2533	rBV	87819	121966	1.40%	0.212%
20	18.016	2533	2538	2546	rVV2	484308	714105	8.19%	1.239%
21	18.157	2557	2562	2566	rBV2	121654	219460	2.52%	0.381%
22	18.198	2566	2569	2575	rVB	70978	102065	1.17%	0.177%
23	18.504	2617	2621	2626	rVB2	62900	89605	1.03%	0.155%
24	18.869	2677	2683	2686	rBV	120234	207708	2.38%	0.360%
25	18.934	2686	2694	2697	rVV3	401629	520174	5.97%	0.902%
26	19.004	2702	2706	2712	rBV3	58932	101706	1.17%	0.176%
27	19.063	2712	2716	2720	rBV	171088	181741	2.08%	0.315%
28	19.122	2721	2726	2731	rBV	811783	1043050	11.96%	1.809%
29	19.251	2745	2748	2756	rBV2	191132	280780	3.22%	0.487%
30	19.475	2777	2786	2795	rBV	813732	1263836	14.50%	2.192%
31	19.681	2816	2821	2826	rBV	7391994	8718926	100.00%	15.125%
32	19.798	2836	2841	2846	rBV5	76848	171532	1.97%	0.298%
33	19.957	2866	2868	2873	rVB	88971	125557	1.44%	0.218%
34	20.063	2882	2886	2890	rBV3	77914	110264	1.26%	0.191%
35	20.116	2891	2895	2899	rVV3	96368	129838	1.49%	0.225%
36	20.251	2915	2918	2921	rBV	90819	101203	1.16%	0.176%

LSC Area Percent Report

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Data File : BP006745.D
Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.298	2922	2926	2933	rVB3	100875	210639	2.42%	0.365%
38	20.692	2990	2993	3000	rVB	91822	126414	1.45%	0.219%
39	20.945	3031	3036	3041	rBV5	391876	670926	7.70%	1.164%
40	21.133	3065	3068	3071	rBV	146821	143601	1.65%	0.249%
41	21.204	3074	3080	3084	rVV2	2238377	3329236	38.18%	5.775%
42	21.239	3084	3086	3093	rVB	476927	585923	6.72%	1.016%
43	22.816	3349	3354	3365	rBV3	412799	1311875	15.05%	2.276%
44	23.316	3436	3439	3446	rVB	255937	418067	4.79%	0.725%
45	23.410	3451	3455	3464	rVB	337403	684922	7.86%	1.188%
46	23.516	3467	3473	3480	rBV2	1337515	2634041	30.21%	4.569%

Sum of corrected areas: 57645401

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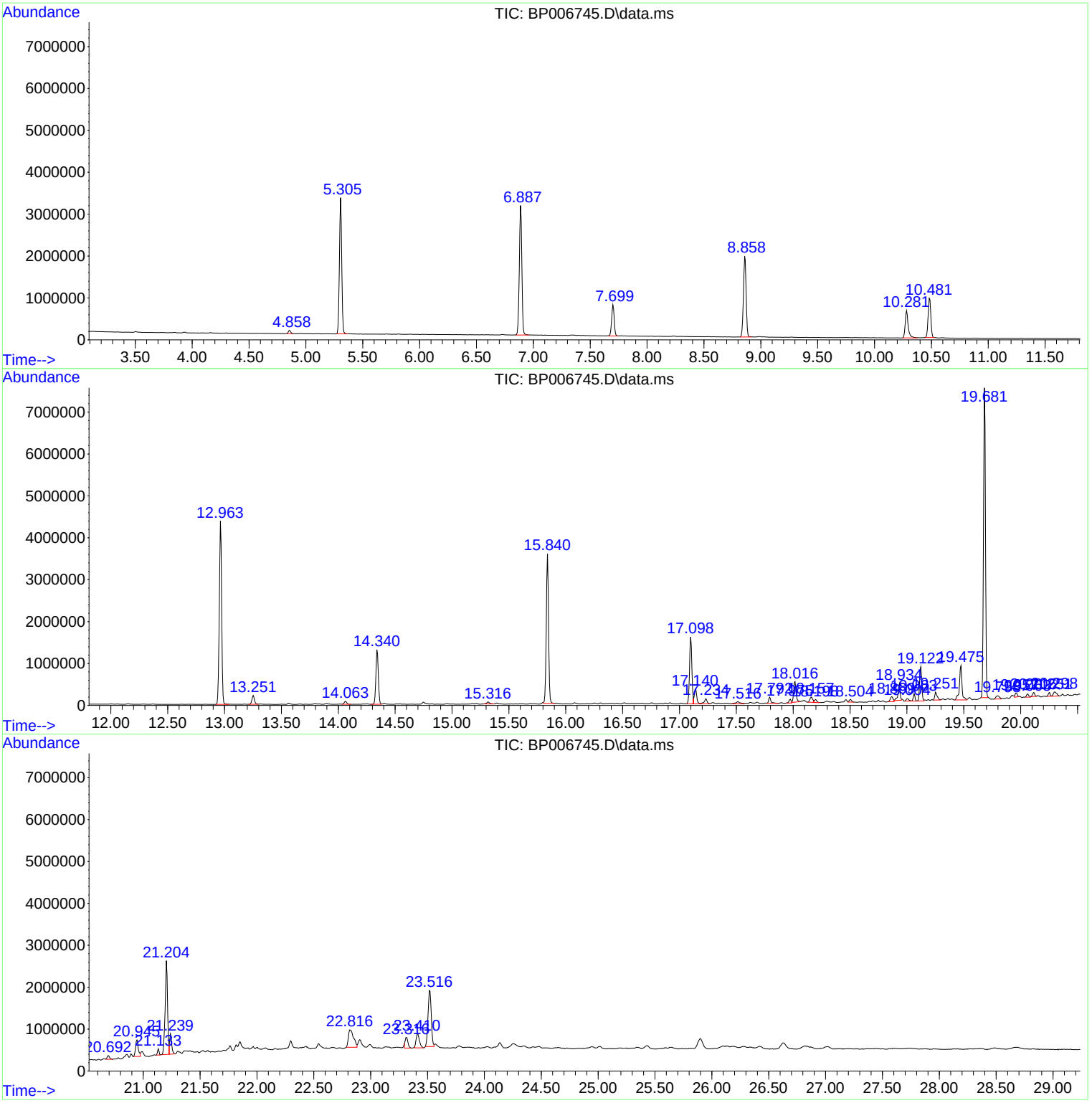
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081821\
Data File : BP006745.D
Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

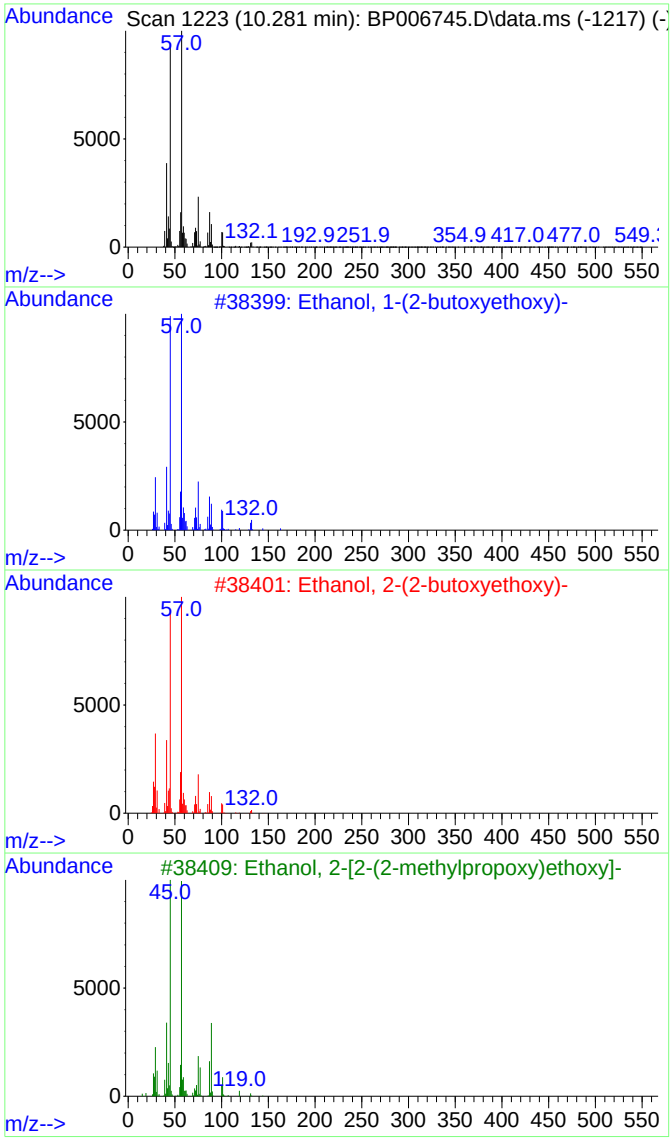
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

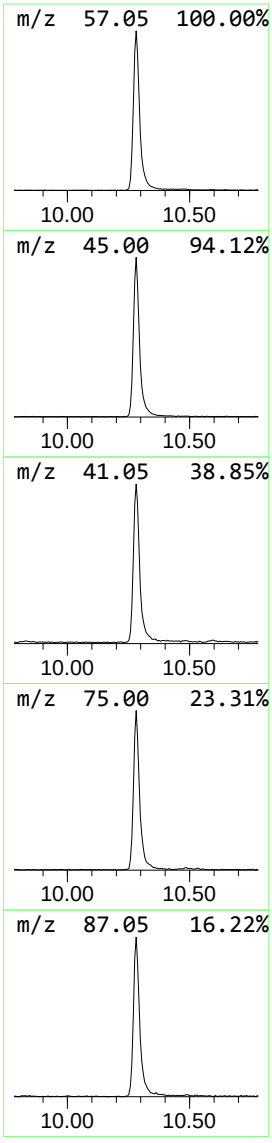
****

Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.281	15.04 ng	1165800	Naphthalene-d8	10.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081821\
Data File : BP006745.D
Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

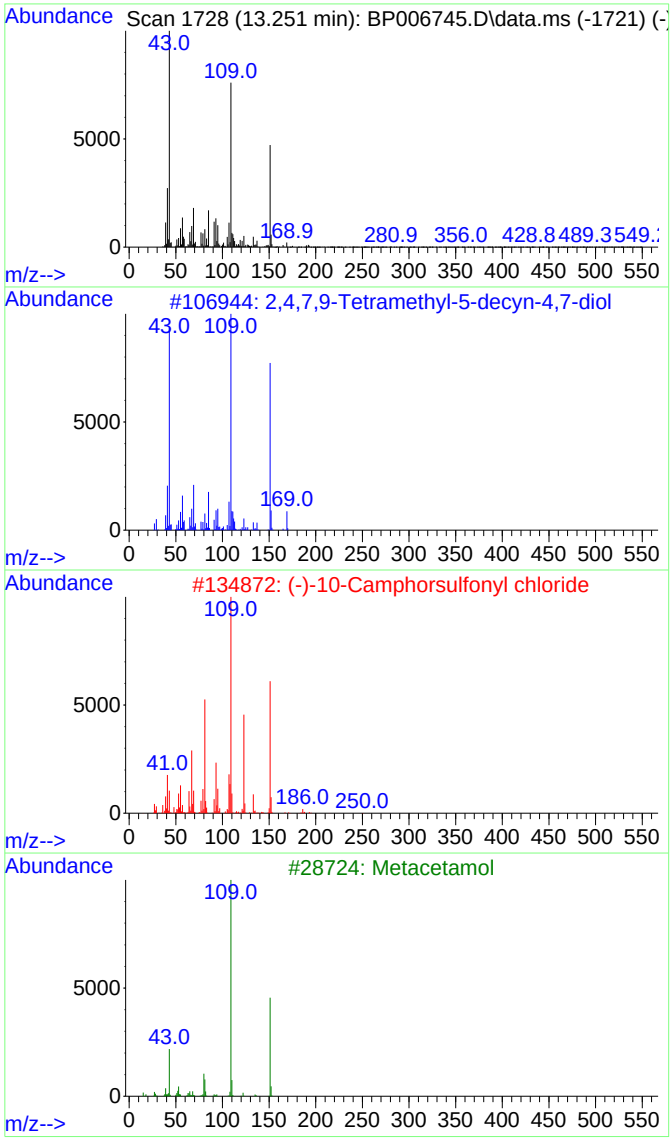
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

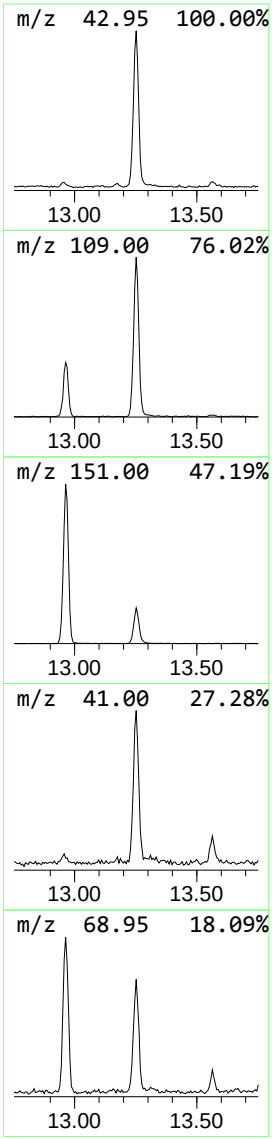
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.252	3.46 ng	333058	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	87
3	Metacetamol	151	C8H9NO2	000621-42-1	58
4	Acetaminophen	151	C8H9NO2	000103-90-2	53
5	Diacetamate	193	C10H11NO3	002623-33-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081821\
Data File : BP006745.D
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Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

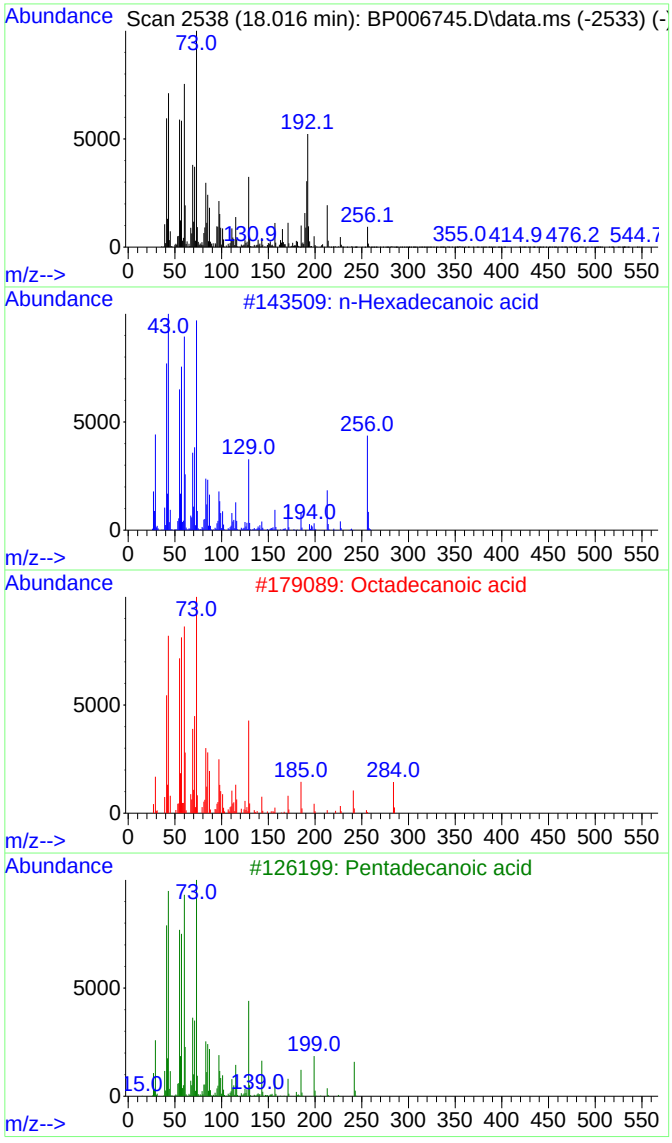
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

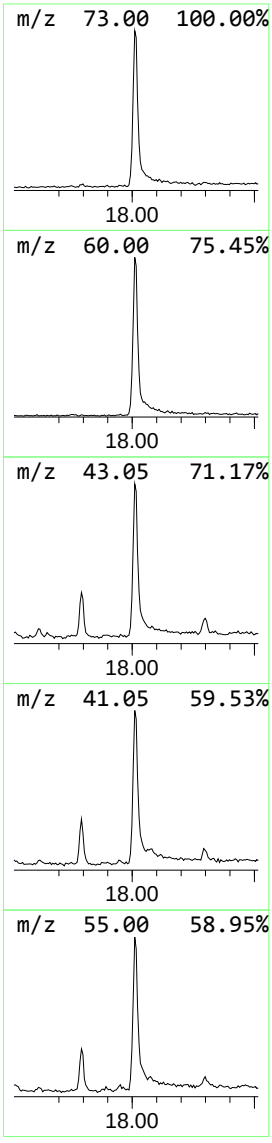
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	6.34 ng	714105	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	56
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081821\
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Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

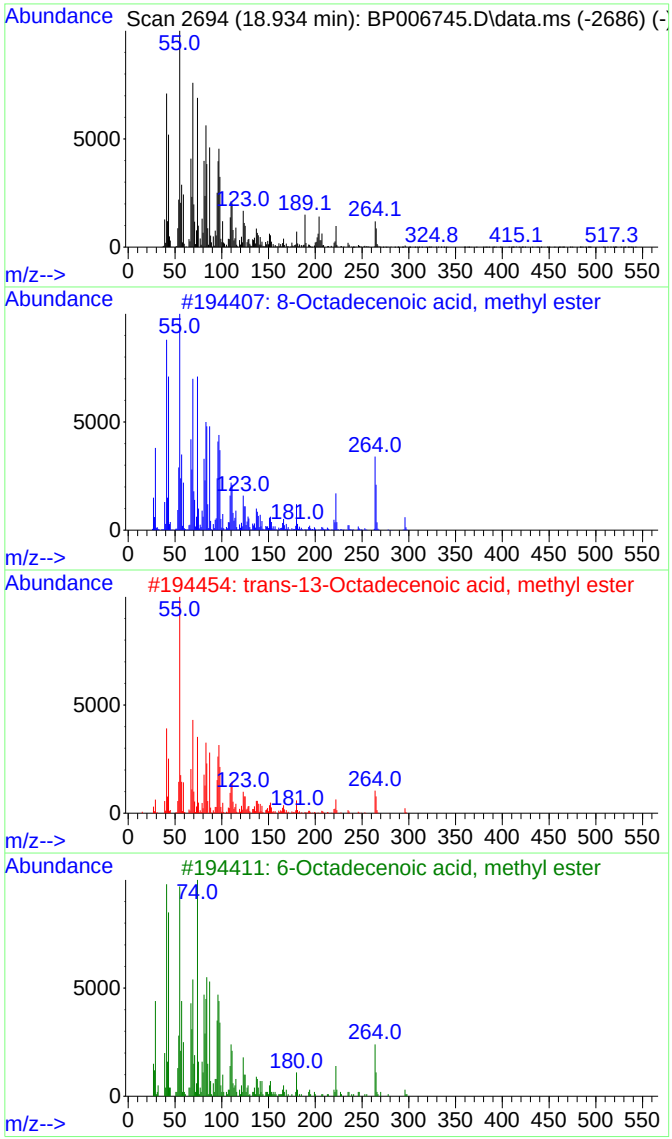
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

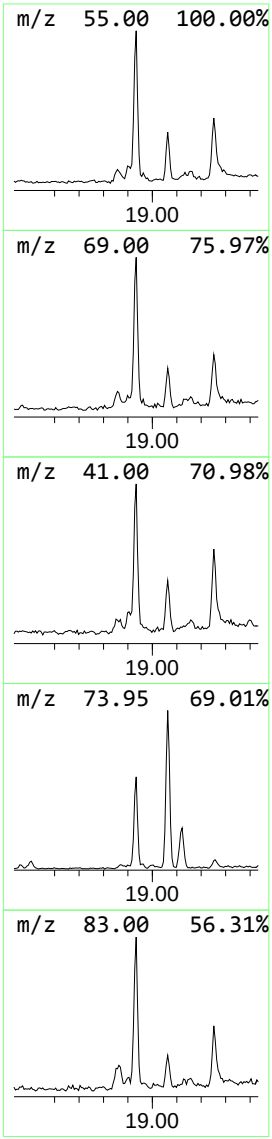
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 8-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.933	4.62 ng	520174	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	98
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	97
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	96





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Acq On : 18 Aug 2021 15:14
Operator : CG/JU
Sample : M3429-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

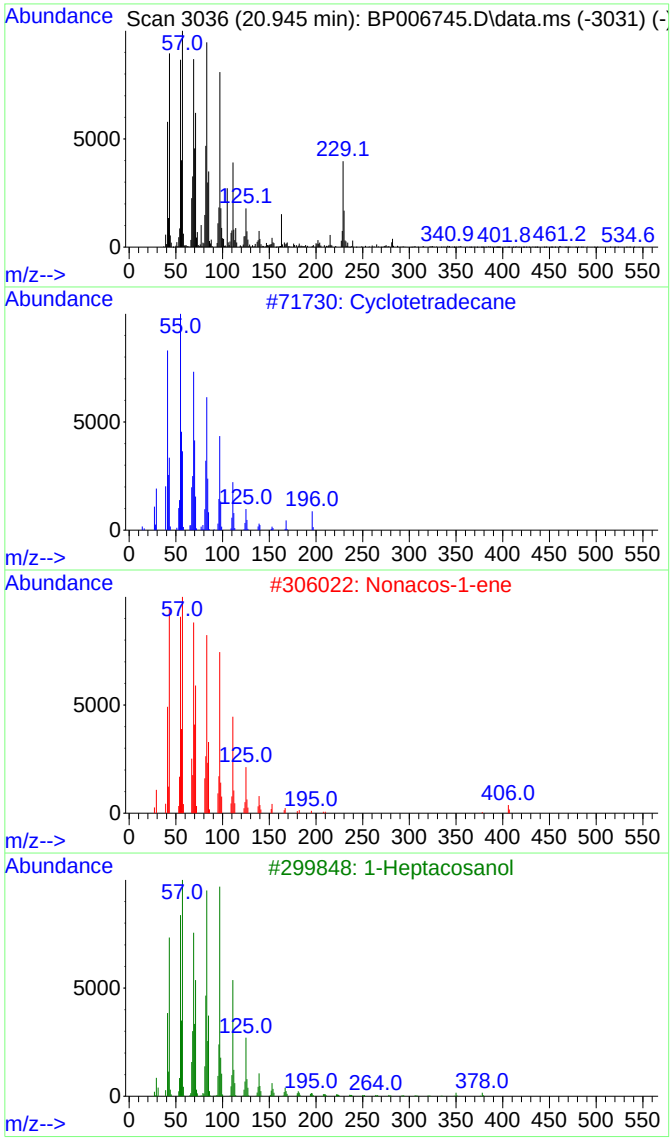
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

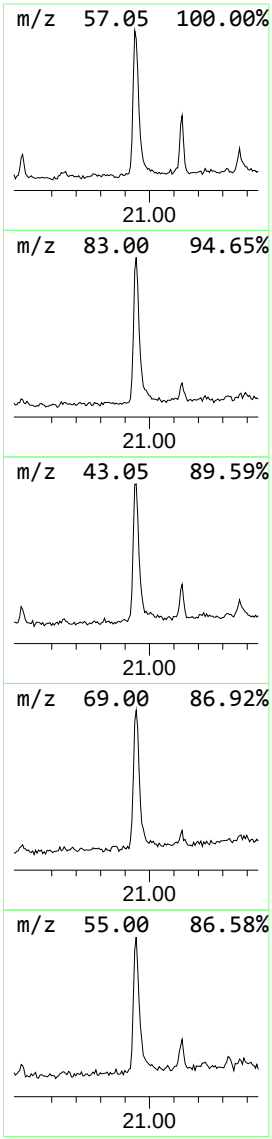
****

Peak Number 5 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	4.03 ng	670926	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	Nonacos-1-ene	406	C29H58	018835-35-3	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

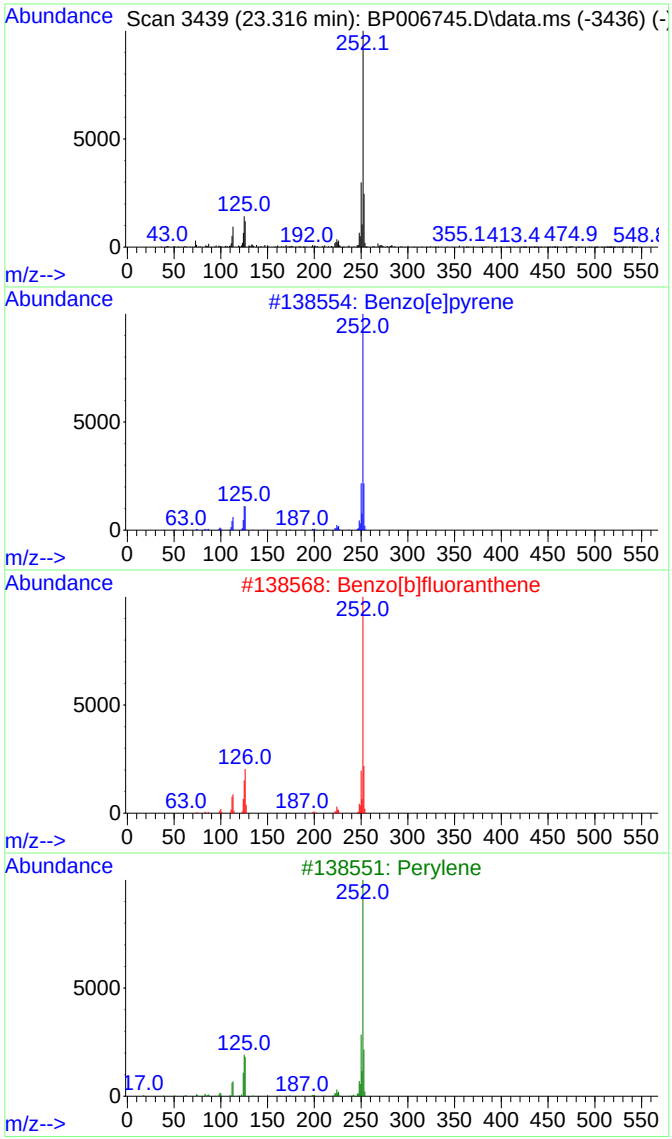
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

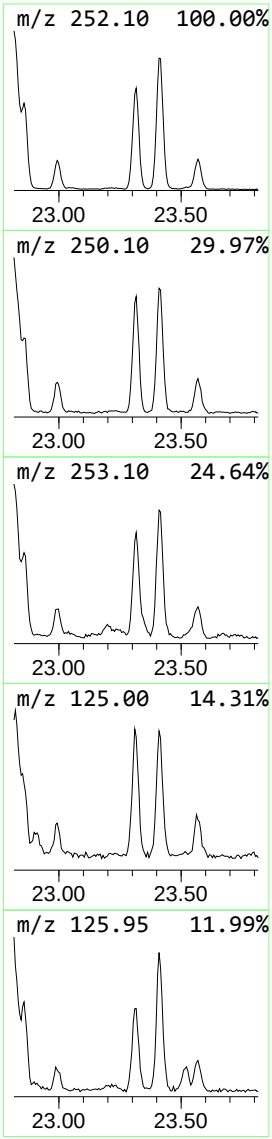
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.316	3.17 ng	418067	Perylene-d12	23.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
3	Perylene	252	C20H12	000198-55-0	91
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 1-(2-b...	10.281	15.0	ng	1165800	2	10.481	1550260	20.0
2,4,7,9-Tetrame...	13.252	3.5	ng	333058	3	14.340	1927380	20.0
n-Hexadecanoic ...	18.016	6.3	ng	714105	4	17.098	2251830	20.0
8-Octadecenoic ...	18.933	4.6	ng	520174	4	17.098	2251830	20.0
Cyclotetradecane	20.945	4.0	ng	670926	5	21.204	3329240	20.0
Benzo[e]pyrene	23.316	3.2	ng	418067	6	23.516	2634040	20.0